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US Army Research Laboratory

Application of High Performance Computing for Simulations of N-Dodecane Jet Spray with Evaporation

by Louis Wonnell, Luis Bravo, and Anindya Ghoshal

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14. ABSTRACT
The problem of turbulent jet sprays of n-dodecane injected into a quiescent nitrogen gas chamber was investigated as a test case for the incorporation of a multiphysics Large-Eddy Simulation solver known as LESLIE into the US Army Research Laboratory's High Performance Computing system. Preliminary simulations were performed on the Excalibur supercomputer to test the capability of the solver to simulate subcritical turbulent jet sprays. The solver was chosen for its ability to make use of alternative models that are capable of modeling multicomponent fluids such as n-dodecane. The long-term goal of this research is to incorporate these models into future simulations of turbulent jet sprays and develop a predictive theory for comparison to measurements in the laboratory of turbulent diesel sprays.

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Student Bio

Impact of High Performance Computing (HPC) Internship Program Research Experience

Prior to this summer's internship, I held 2 Master's degrees in Mechanical and Nuclear Engineering. I had focused on plasma physics at the University of California, San Diego, but the bulk of my research was in Computational Fluid Dynamics at North Carolina State University and Kansas State University. I was simulating turbulent incompressible and compressible flows, and the collaboration between my advisor and Dr Luis Bravo led to my internship at the US Army Research Laboratory (ARL).

I did not know what to expect at ARL, having neither done a summer internship at a research laboratory, nor having any experience working with the Military. The staff and researchers all made me feel at home both in the lab and during social events. The tough stages of obtaining and processing paperwork were made easier by the assistance of every level of staff.

For the research, I expected to be challenged by the size and scope of a new industrial code, and my work with the LESLIE code clearly lived up to those expectations. The scope and size of modules available in LESLIE made clear what kinds of efforts went into typical industrial codes. Luckily, the process of installing and running the code went without major hurdles, due in large part to the help of the Georgia Institute of Technology staff.

The preliminary simulations I performed with turbulent jet sprays will likely continue as Dr Bravo and my advisor, Dr Chen, collaborate with our Morphing Continuum Theory at Kansas State University. We are looking to better predict turbulent physics within compressible flows, which require good predictions of the thermodynamics of the flow. Dr Chen gave a lecture regarding this topic at ARL recently; therefore, there does seem to be interest in working together in the future. I would be glad to work with Dr Bravo in the future, as he has been a window into the larger world of fluid physics research as it applies to the Military.

Acknowledgments

I would like to thank Dr Luis Bravo for being a most helpful mentor while I was at the US Army Research Laboratory (ARL) and for accepting me. I would like to thank Dr Chen for supporting my decision to apply for an internship at ARL and for supporting me at Kansas State University. I would like to thank Deborah Stowell for her help and assistance escorting us on base. Finally, I would like to thank my coworkers, and particularly my roommates, Kathryn Esham and Richard Blocher.

1. Summary

The problem of turbulent jet sprays of n-dodecane injected into a quiescent nitrogen gas chamber was investigated as a test case for the incorporation of a multiphysics Large-Eddy Simulation solver known as LESLIE into the US Army Research Laboratory's (ARL's) High Performance Computing (HPC) system. Preliminary simulations were performed on the Excalibur supercomputer to test the capability of the solver to simulate subcritical turbulent jet sprays. The solver was chosen for its ability to make use of alternative models that are capable of modeling multicomponent fluids such as n-dodecane. The long-term goal of this research is to incorporate these models into future simulations of turbulent jet sprays and develop a predictive theory for comparison to measurements in the lab of turbulent diesel sprays.

The results obtained in this study were compared with experimental measurements of real turbulent jet sprays by the Institute Francais du Petrole Energies Noivelles (IFPEN).[1] Visualizations of the contour plots in the domain were obtained using ParaView, showing the formation of individual eddies in temperature, density, and velocity contours. The lack of evaporation in the domain is demonstrated by the comparison with experimental data. Numerical results show a 3 mm increase in the drop of mean liquid length when compared with experiments obtained by IFPEN.[1]

2. Introduction

A critical component of maintaining performance and durability of a diesel engine involves the formation of a fuel-air mixture as a diesel jet spray mixes with a quiescent gas chamber. When the liquid fuel interacts with the quiescent gas, turbulent mixtures form and may even combust. Obtaining a better understanding of the flow characteristics of the mixture and combustion processes will help improve emissions and aid the military in choosing a single fuel that will reduce the payload for all of its diesel-powered vehicles, including unmanned aerial vehicles.[2]

A consistent problem in conducting this research involves producing clear images and reliable data of the fuel-air mixture at each stage of its development at reasonable costs. New methods involving X-rays and ballistic imaging of the near field in a diesel spray and the use of medical imaging have observed the liquid core or near-nozzle behavior of spray-vapor mixtures.[3,4] When the spray becomes optically dense, these X-ray techniques have been the only effective way of capturing 3-D, time-averaged images of the primary breakup region of optically dense sprays.[4] Still, a full 4-D description of the optically dense regions of the

spray, with the spatio-temporal resolution required for a detailed analysis, has yet to be achieved.[5]

Therefore, to obtain better data for these fuel mixtures, the research community has looked to numerical solvers designed to incorporate turbulence models as well as thermodynamic equations to handle evaporation or combustion in the spray. Bharadwaj et al. performed Large-Eddy Simulations (LES) on nonevaporating sprays featuring large numbers of particles and they found good agreement with X-ray experiments done by Argonne National Lab.[6] The study demonstrated that LES could model 2-phase flows as well as track the effects of subgrid scales on turbulent kinetic energy.

In the simulations of more complex fluid mixtures, however, current numerical results have relied on simpler thermodynamic equations of state designed for binary mixtures and flows where the liquid and vapor phases could easily be distinguished. Current problems in turbulent jet sprays involve multicomponent fluids, where the fuel-mixture is composed of several different compounds. Dahms and Ofelein derived equations of state for multicomponent fluids based on Gradient Theory.[7] The theory determined the significance of factors—such as surface tension, mean-free path, and the liquid-vapor interface—to the overall behavior of the mixture. Still, the complex model had the drawback of remaining computationally inefficient.[7]

The demand remains for a flexible multiphysics solver capable of simulating turbulent jet sprays composed of multicomponent fluids without incurring high computational costs. For this research, preliminary steps of obtaining this solver were performed. A multiphysics solver known as LESLIE was incorporated into the ARL HPC system. The solver relied on particle-based LES methods, and came equipped with several different turbulence and thermodynamics models. In particular, a real-fluids model known as the Peng-Robinson model will allow for more realistic modeling of these multicomponent fuels. For this research, the solver was tested for subcritical n-dodecane fuels injected into a quiescent chamber of 100% nitrogen gas. Critical parameters were measured for chamber temperatures ranging from 700 to 1000 K and compared with experimental results. In addition, test simulations for numbers of particles and processors were performed to gauge how well the code performed when default parameters were altered. The basics of the LESLIE code and the test case parameters are briefly described in Section 3. Section 4 presents the comparison of numerical results to experimental results, and ParaView contour plots of density, velocity, and temperature of the jet spray. Section 5 summarizes the progress obtained with the code and the next steps involved in future simulations with LESLIE.

3. Methods, Assumptions, and Procedures

The LESLIE solver comes equipped with finite volume and finite difference schemes of various orders. The simulations for this research made use of MacCormack's Method, which combined the 2 approaches. Finite volume equations were solved to obtain solutions to the Euler equations, while the viscous fluxes were solved using a finite-difference approach. The Eulerian fluxes at the face were extrapolated from the cell-averaged values at the interior, while the viscous fluxes are determined from the grid. Governing equations, filtering processes, and turbulence model details for the LESLIE code are all specified in detail in the LESLIE manual.[8]

All of the simulations were performed in a rectangular prism of 10-mm width and height and a 100-mm length, with the material and mesh parameters listed in Table 1. A slice of the mesh is visible in Fig. 1, giving a sense of the relative uniformity of the mesh. Figure 2 shows a distribution of the edge ratios of the mesh. The edge ratios remained low for a large majority of the cells. Figures 3–5 indicate the Jacobian, Skew, and Stretch values for the mesh. Low orders of magnitude indicate relatively little alteration in the cells across the domain, with most of the deformation occurring near the nozzle.

Table 1 Initial values for fuel, chamber, and mesh. Parcel numbers were altered for parcel sensitivity simulations.

Parameter	Value
v_inject	450 m/s
n_cells	4059072
n_points	4666368
n_blocks	384
Time step	4.00E-09 s
r_parcel	4.50E-05 m
n_parcels	632
r_nozzle	4.50E-05 m
m_rate	.00233 kg/s
T_fuel	363 K
ρ_fuel	22.8 kg/m^3

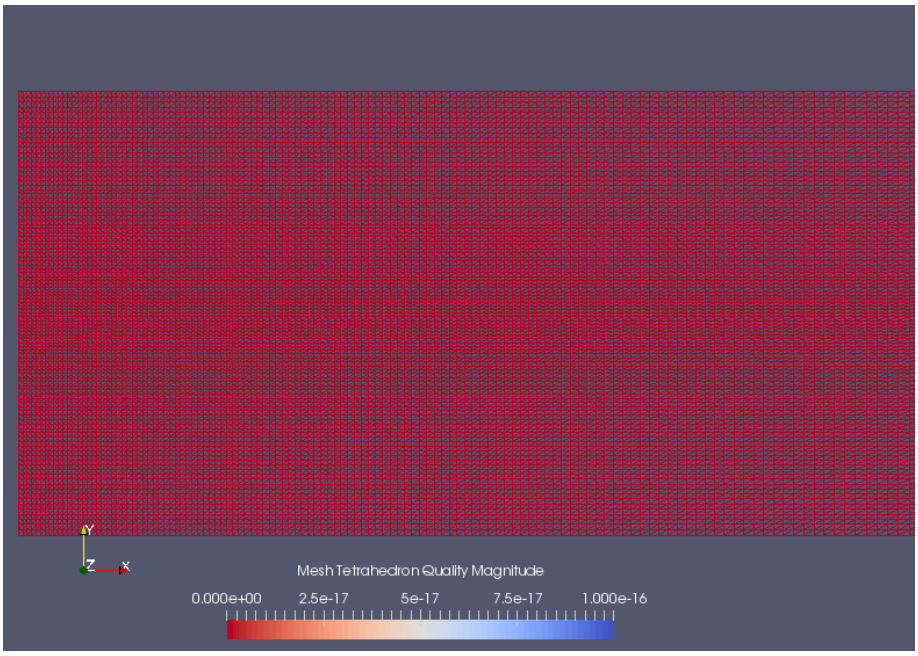

Fig. 1 Image of slice of mesh, showing relative uniformity of cell shapes

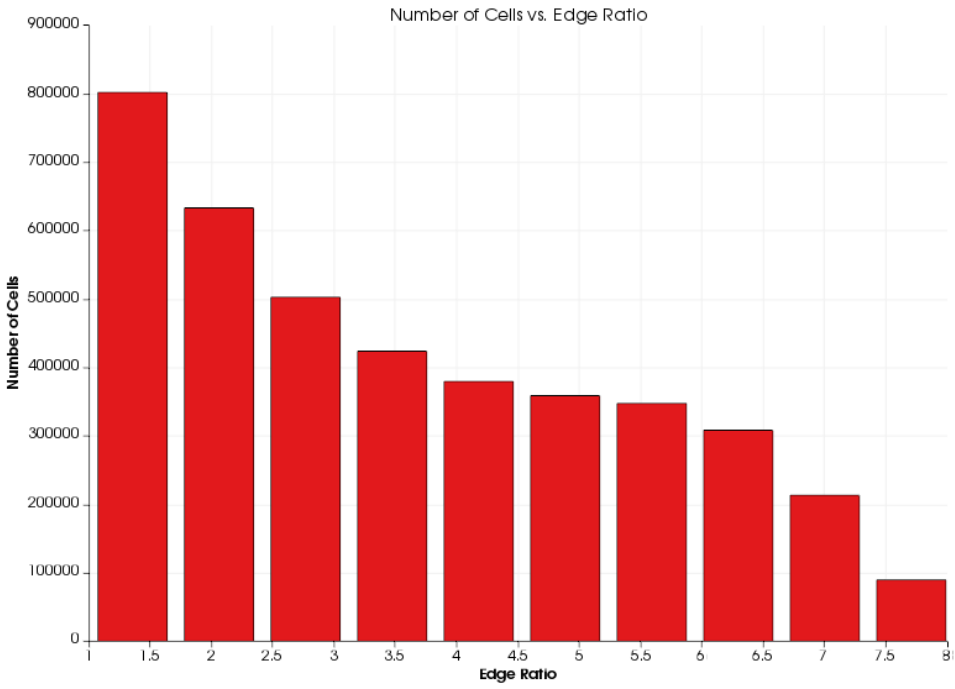

Fig. 2 Distribution of edge ratio in mesh

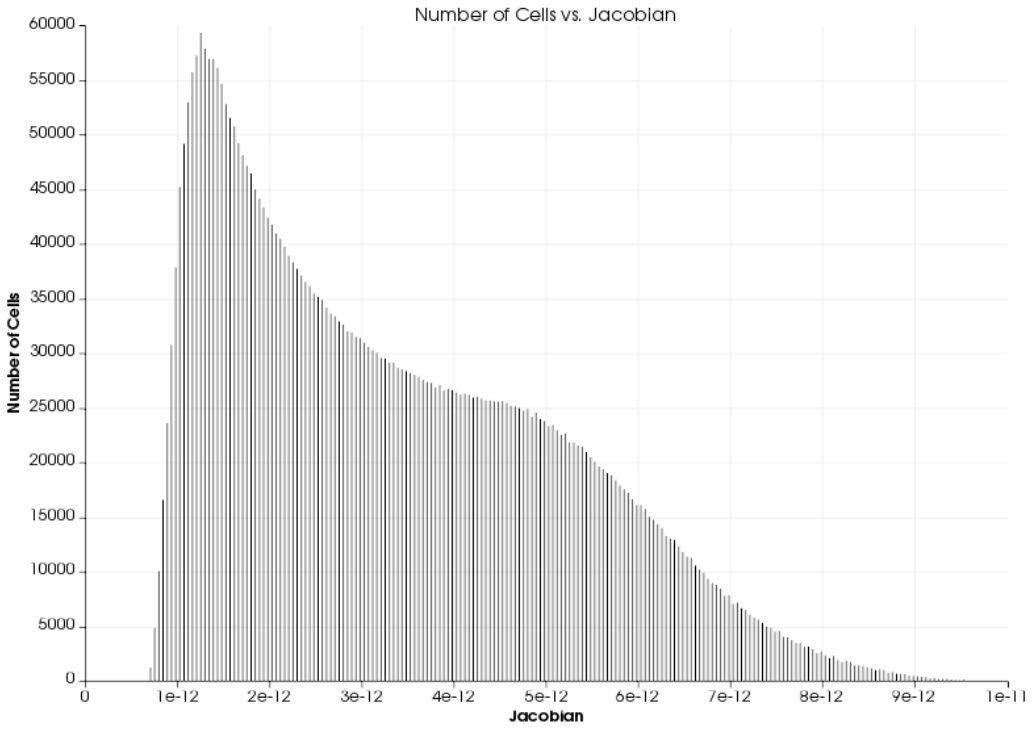

Fig. 3 Distribution of Jacobian value in mesh

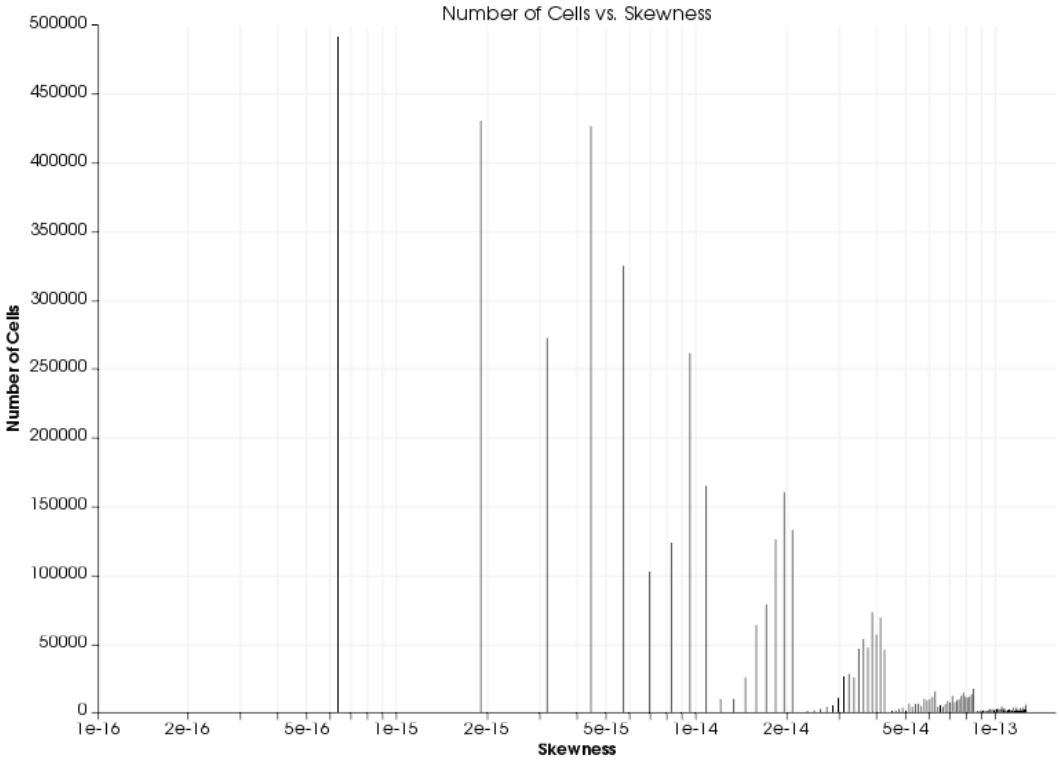

Fig. 4 Distribution of skewness in the mesh

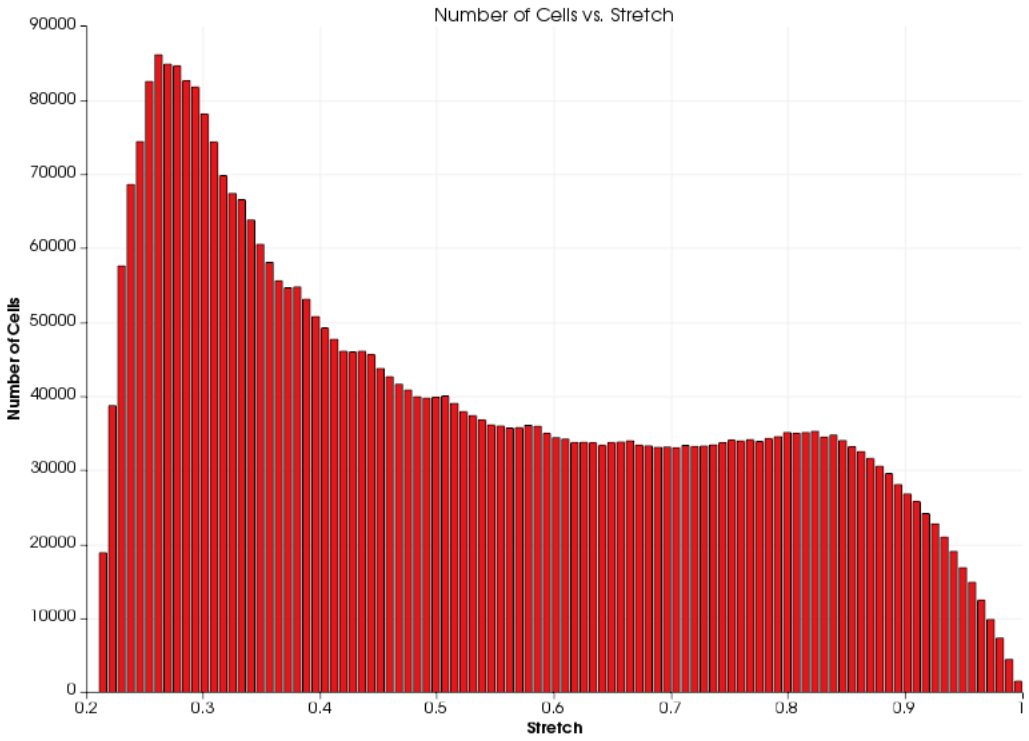

Fig. 5 Distribution of stretch in the mesh

For this simulation, the dodecane spray was assumed to be subcritical. Therefore, evaporation was not considered in the equations of state governing the thermodynamics. It was predicted, therefore, that the liquid penetration length would be overestimated in comparison with the experimental results. Parcel sensitivity studies were done with the radius of the injected parcels reduced by 2 in each simulation. The larger numbers of parcels would hopefully yield a higher resolution of the contour slice and reduce the fluctuations in the liquid length.

4. Results and Discussion

The numerical data are summarized in Figs. 6 and 9. The predicted overestimation of the liquid length due to the lack of evaporation in the thermodynamic equations of state is clearly demonstrated in Fig. 6 for chamber temperatures of 800 to 1000 K. The trend in evolution of the liquid length, however, is similar to the IFPEN results, so the effects of chamber temperature appear to be captured. Figure 10, meanwhile, shows the liquid length behavior from the parcel sensitivity study. When the parcel radius was reduced to half of the original radius, the oscillations about the numerical mean decreased and the liquid length began to stabilize. After the parcel radius was reduced to a quarter of the original radius, however, the oscillations picked up again. A more detailed study would show whether this trend

would occur for all chamber temperatures and whether it is a sign of numerical instability. Figures 7–10 show a comparison of the contour slices for the half-sized and quarter-sized parcel simulations at 900 K at a time of 1 ms. Some of the diffuse spray appears to disappear for the quarter-sized parcel simulations, but the simulations do not appear to match each other in behavior regardless. It is possible that the spike in parcel number associated with the quarter-sized simulations allowed for spikes in the liquid ratio out by the edge of the spray.

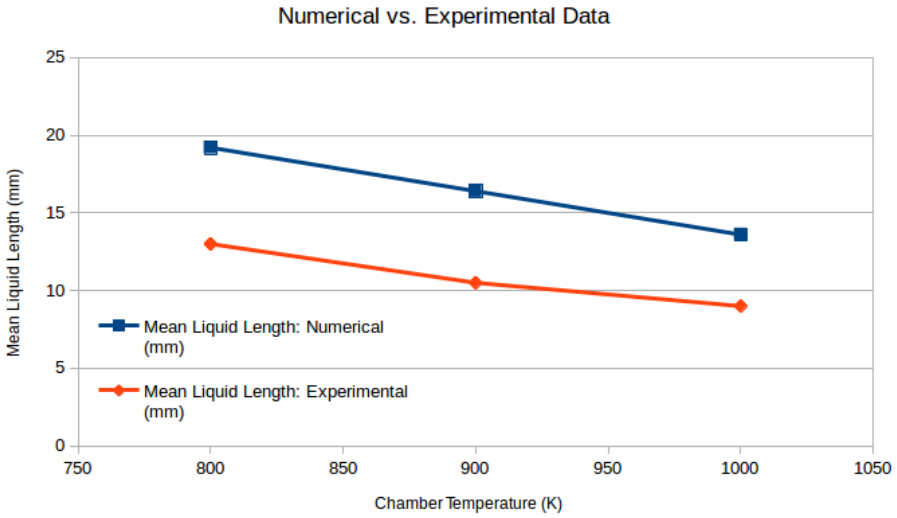

Fig. 6 Comparison of liquid length data between numerical and experimental data (IFPEN 2013). Consistent overestimation of liquid length in numerical results likely due to subcritical mixture assumption.

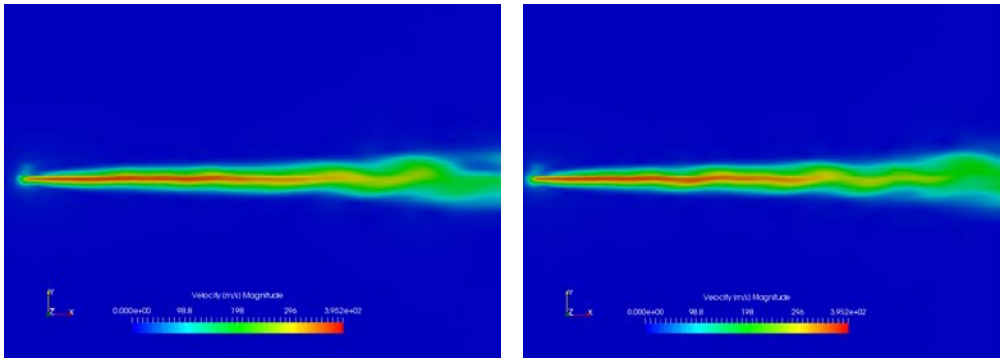

Fig. 7 Velocity slice comparison, T_chamb = 900 K, Left: r_parcel = 0.5*r_initial, Right: r_parcel = 0.25*r_initial, t = 1 ms

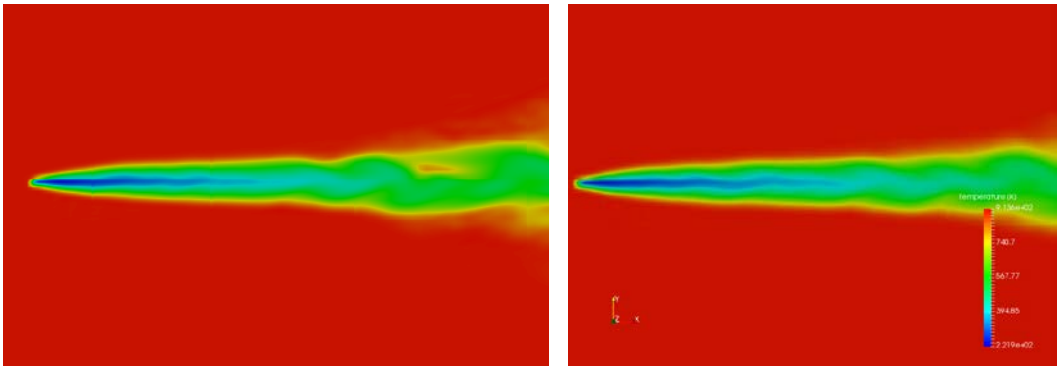

Fig. 8 Temperature slice comparison, T_chamb = 900 K, Left: r_parcel = 0.5*r_initial, Right: r_parcel = 0.25*r_initial, t = 1 ms

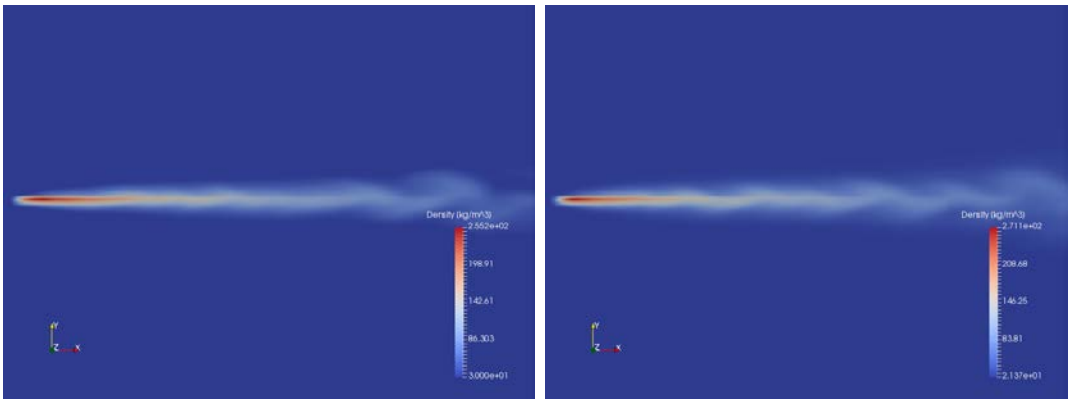

Fig. 9 Density slice comparison, T_chamb = 900 K, Left: r_parcel = 0.5*r_initial, Right: r_parcel = 0.25*r_initial, t = 1 ms

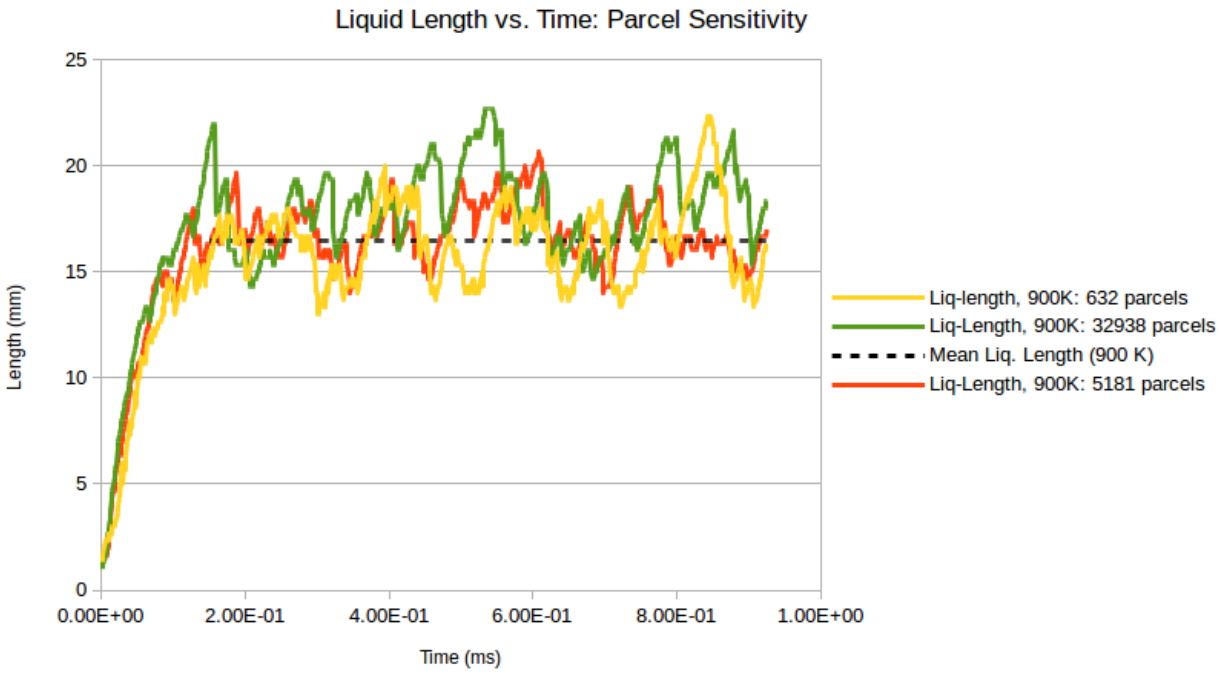

Fig. 10 Liquid length (mm) measurements for T_chamb = 900 K for n_parc = 632 (r_parc = r_initial), 5 k (r_parc = 0.5*r_initial), and 32 k parcels (r_parc = 0.25*r_initial). Fluctuations decrease at 5 k parcels but pick back up with 32 k parcels.

5. Conclusion

The preliminary results from the first few simulations of the LESLIE code do not yield surprising results. The trend in liquid penetration length with chamber temperature matches closely with experimental data, but overshoots the experiments likely due to the lack of evaporation. With the real fluids models currently built into the LESLIE code, future simulations should be able to determine whether other factors influence this disparity. The more interesting results come from the parcel sensitivity data, as the oscillations begin to emerge again with the quarter-sized parcels. Data for simulations with parcel sizes even smaller than quarter-sized parcels were not shown as these led to instabilities in the solver; therefore, it appears that the code is highly sensitive to the number of parcels present. The results from the quarter-sized parcels, therefore, may deviate from physically reliable data. Still, preliminary simulations indicate that the LESLIE code is ready for future simulations to compare with more available experimental data as it arrives.

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List of Symbols, Abbreviations, and Acronyms

3-/4-D	3-dimensional/4-dimensional
ARL	US Army Research Laboratory
HPC	High Performance Computing
IFPEN	Institute Francais du Petrole Energies Noivelles
K	Kelvin
LES	Large-Eddy Simulation

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